

THE THREE-BODY CONTINUUM COULOMB PROBLEM AND THE 3α STRUCTURE OF ^{12}C

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Abstract

We introduce an approach, based on the coordinate space Faddeev equations, to solve the quantum mechanical three-body Coulomb problem in the continuum. We apply the approach to compute measured properties of the first two 0^+ levels in ^{12}C , including the width of the excited level, in a 3α -particle model. We use the two-body interaction which reproduces the low energy α - α scattering data and add a three-body force to account for the compound state admixture.

Introduction. The quantum mechanical three-body problem with Coulomb interaction is yet one of the unsolved problems of few body physics (see, for example, [1, 2, 3, 4]). A number of three-body Coulomb problems in nuclear, atomic and molecular physics cannot be dealt with at the moment because of the principal difficulties in constructing correct asymptotic wave functions in the case when none of the two body subsystems is bound.

One of such problems is the description of the astrophysically significant second 0^+ state in ^{12}C (denoted 0_2^+) as a system of three alpha particles [5, 6]. Despite the long history of investigations it is yet unclear to what extent the three-body picture accounts for the real structure of this state as it lies above the threshold and requires therefore correct continuum spectrum solutions of the three-body Coulomb problem.

The purpose of this letter is two-fold. First we introduce an approach to compute the three-body continuum spectrum for Coulomb interactions. We construct the asymptotic functions employing the adiabatic hyperspherical expansion of the coordinate space Faddeev equations [7]. This method proved to be very powerful in treating the long-distance behavior of three-body systems including the pathological Efimov effect [8]. The approach is a generalization of the adiabatic hyperspherical method, successfully used in atomic physics [9], into the more versatile Faddeev equations.

Secondly, we apply the invented method to the two lowest 0^+ states in ^{12}C where descriptions in terms of three interacting α -particles traditionally are believed to be rather accurate. The second state 0_2^+ is unbound with respect to three free α -particles and its structure (along with the ground state structure) has been debated for many years, see for example [10, 11, 12]. A correct description, which must include continuum effects of the long-range Coulomb interaction, is therefore now possible.

As repeatedly suggested we shall include a genuine three-body force in order to account for three-body effects related to the Pauli principle and polarization effects [13]. Beside providing information about the structure, the method also enables us to give an estimate of the width of the 0_2^+ -level within the genuine three-body model.

Method. We solve the Faddeev equations in coordinate space using the adiabatic hyperspherical expansion method [7, 14]. We shall use hyperspherical coordinates, which consist of one radial coordinate ρ (hyperradius) and five generalized angles denoted by Ω . The hyperradius ρ is defined in terms of the center of mass coordinates of the α -particles r_i as $\rho^2 = A_\alpha \sum_{i=1}^3 r_i^2$, where $A_\alpha = m_\alpha/m = 3.97$ is given by the nucleon mass m and the α -particle mass m_α .

For a fixed ρ we consider the eigenvalue equation for the five dimensional spin-angular part of the Faddeev operator, i.e.

$$\left(T_\Omega - \lambda_n\right)\Phi_{n,(i)}^{JM} + \frac{2m}{\hbar^2}\rho^2 V_i \Phi_n^{JM} = 0, \quad i = 1, 2, 3, \quad \Phi_n^{JM} = \Phi_{n,(1)}^{JM} + \Phi_{n,(2)}^{JM} + \Phi_{n,(3)}^{JM}, \quad (1)$$

where T_Ω is the angular part of the kinetic energy operator and V_i is the potential between particles j and k , where $\{i, j, k\}$ is a cyclic permutation of $\{1, 2, 3\}$. The eigenvalues $\lambda_n(\rho)$ and the eigenfunctions $\Phi_n^{JM}(\rho, \Omega)$, which also carry the dependence of the spins of the particles, are calculated as function of ρ . The total three-body wave function is then expanded in terms of these eigenfunctions, i.e.

$$\Psi^{JM} = \frac{1}{\rho^{5/2}} \sum_n f_n(\rho) \Phi_n^{JM}(\rho, \Omega). \quad (2)$$

The system of coupled hyperradial equations for the expansion coefficients $f_n(\rho)$ finally becomes

$$\left(-\frac{d^2}{d\rho^2} - \frac{2mE}{\hbar^2} + \frac{15/4}{\rho^2} + \frac{\lambda_n(\rho)}{\rho^2}\right)f_n(\rho) = \sum_{n'} \left(2P_{nn'}\frac{d}{d\rho} + Q_{nn'}\right)f_{n'}(\rho), \quad (3)$$

$$P_{nn'}(\rho) = \int d\Omega \Phi_n^* \frac{\partial}{\partial \rho} \Phi_{n'}, \quad Q_{nn'}(\rho) = \int d\Omega \Phi_n^* \frac{\partial^2}{\partial \rho^2} \Phi_{n'}.$$

For large ρ the non-diagonal terms P and Q are small compared to the diagonal terms $\lambda_n(\rho)$ which, divided by ρ^2 , serve as an effective adiabatic hyperradial potential.

The large distance tail of the eigenvalues $\lambda_n(\rho)$ is independent of the properties of the short-range nuclear force. The derivation of this asymptotic behavior is difficult and beyond the scope of this letter, but the result can be written as [15]

$$\lambda_n(\rho \rightarrow \infty) \rightarrow 3\eta\rho + C_n\sqrt{\eta\rho} + \dots, \quad (4)$$

where $\eta = \frac{2m}{\hbar^2}(2e)^2\sqrt{A_\alpha}$, $2e$ is the charge of the α -particle and C_n are constants. For the lowest term this constant is $C_1 = 9/4$. At large distances the adiabatic potential λ_n/ρ^2 has therefore a Coulomb term $3\eta/\rho$, with the next term behaving as $\rho^{-3/2}$. These terms are absent for uncharged particles.

For a positive energy $E \equiv \hbar^2\kappa^2/(2m)$ the general solution of equation (3) asymptotically is a linear combination of two linearly independent solutions $\exp(\pm i(\kappa\rho - \frac{3\eta}{2\kappa} \log \kappa\rho))$. A resonance with energy E_r and width Γ corresponds to a solution of the system (3) with the complex energy $E_0 = E_r - i\Gamma/2$ [16]. This solution satisfies the boundary condition

$$f_n(\rho \rightarrow \infty) \rightarrow \exp(+i(\kappa_0\rho - \frac{3\eta}{2\kappa_0} \log \kappa_0\rho)), \quad (5)$$

where $\kappa_0 = \sqrt{2m(E_r - i\Gamma/2)/\hbar^2}$. This boundary condition determines that the S -matrix has a pole at the complex energy E_0 .

Interactions. We use the Ali-Bodmer potential version "a" [17] slightly altered to reproduce the s-wave resonance of ^8Be at 0.093 MeV in addition to the low energy $\alpha\alpha$ phase shifts. The potential is given as

$$V = (125\hat{P}_{l=0} + 20\hat{P}_{l=2})e^{-r^2/1.53^2} - 30.18 e^{-r^2/2.85^2}, \quad (6)$$

where lengths and energies are in units of fm and MeV, respectively. The \hat{P}_l is the projection operator onto the state with relative orbital angular momentum l .

It is well known that this potential underbinds the 0^+ states [10] due to the strong repulsive core which is necessary to simulate the Pauli repulsion in the 2α system. The width of the resonance depends crucially on its energy, and to estimate this width accurately we need the resonance energy at the correct position. We achieve this by introducing an additional attraction.

Indeed, when three α -particles are close together one of them polarizes the other two beyond the polarization included in the two-body interaction. Thus the Pauli repulsion between them should be reduced. This effect can be imitated by a phenomenological three-body attractive force, which must be non-vanishing

only when all three particles are close together, that is for small ρ . This “off shell” effect must disappear at large ρ where the “on shell” properties of the phase fitted interactions provide the correct asymptotic behavior. As a novel feature we include this additional interaction by parametrizing the three-body potential as a simple gaussian, $V_3(\rho) = S_3 \exp(-\rho^2/b_3^2)$, which is added directly in the hyperradial equations (3).

The strength and the range parameters S_3 and b_3 are now adjusted to reproduce the position of the 0_2^+ level at 0.38 MeV and in addition to get the ground state energy as close as possible to the observed value of -7.27 MeV. This requirement uniquely specifies the range and the strength of the three-body force. The resulting parameters are given in table 1.

Properties of the system. The model is now completely defined and we can compute various measured properties of these two 0^+ states. The crucial quantity is the effective potential in the hyperradial equation, i.e. $W_n \equiv \hbar^2/(2m)((\lambda_n + \frac{15}{4})/\rho^2 - Q_{nn})$ which is shown in fig. 1. The position of the 0_2^+ level is indicated by the dashed line. The combined effect of the three-body centrifugal and Coulomb forces creates a strong barrier extending approximately from 13 to 60 fm. This barrier is responsible for the extremely small width of the resonance.

The **root mean square radius** is in the three-body model given by

$$R_{rms} = \sqrt{R_\alpha^2 + \frac{1}{3A_\alpha} \langle \rho^2 \rangle}, \quad \langle \rho^2 \rangle = \sum_n \int_0^\infty f_n^2(\rho) \rho^2 d\rho, \quad (7)$$

where $R_\alpha = 1.47$ fm is the root mean square radius of the α -particle. As seen in table 1 we underestimate the radius slightly in contrast to a larger overestimate found in other three-body calculations. This difference is due to the attractive three-body force which tends to decrease the size of the system.

The **monopole matrix element** is written as

$$M = 2 \sum_{i=1}^3 \langle 0_{gs}^+ | r_i^2 | 0_2^+ \rangle = \frac{2}{A_\alpha} \langle 0_{gs}^+ | \rho^2 | 0_2^+ \rangle = \frac{2}{A_\alpha} \sum_n \int_0^\infty f_n^{(gs)}(\rho) f_n^{(ex)}(\rho) \rho^2 d\rho, \quad (8)$$

where $f_n^{(gs)}(\rho)$ and $f_n^{(ex)}(\rho)$ are the radial wavefunctions for the ground state and the excited state, respectively. The numerical result given in table 1 is found with the wavefunction for the excited state 0_2^+ calculated as a true bound state by using an infinite wall at 30 fm. We overestimate the matrix element significantly less than other calculations indicating that we obtain a rather good description of the spatial configurations of the two 0^+ levels.

To estimate the **width** of the 0_2^+ state we first use the quasiclassical approximation, that is calculate the penetrability of the combined centrifugal and Coulomb barrier in the lowest adiabatical channel. The penetration factor ($\sim 10^{-4}$) is multiplied by the number of assaults per unit time on the barrier (\sim

1 MeV/ \hbar) computed as the average radial velocity divided by two times the width of the potential well. In this approximation the width is about 100 eV. It is already extremely narrow compared to the resonance energy of 0.38 MeV, although still an order of magnitude larger than the experimental value. The main source of the underestimate is in the neglect of the higher adiabatical channels, especially the second one which has an attractive pocket at $\rho \approx 10$ fm, see fig.1.

We now find the complex energy solution of the system (3) with the boundary condition (5). In order to obtain a converged result we have to integrate the radial equations numerically up to $\rho \approx 80$ fm. As we can solve numerically the Faddeev equations (1) only until $\rho \approx 40$ fm, we have to extrapolate the eigenvalues according to equation (4). Because of the low-lying ^8Be resonance the uncertainty in the third term of the asymptotic expansion leads to an uncertainty in the width of about 10 eV. Within this uncertainty the resulting width is $\Gamma=20$ eV which is remarkably close to the experimental value.

The width of the 0_2^+ level in ^{12}C has also been considered using a two-body $^8\text{Be}+\alpha$ approximation within the α -cluster model (see, for example, [18]). In this approximation the ^{12}C first decays into ^8Be and an α -particle, then ^8Be in turn decays into two α -particles. In our genuine three-body approach the decay proceeds directly into the three-body continuum and the narrow resonance ^8Be comes into play implicitly through the structure of the angular eigenfunctions and eigenvalues.

The **spatial shapes** of the states are somewhat difficult to visualize due to the symmetry of the three particles. The wavefunction depends on six coordinates, which conveniently now can be chosen as the distance between two of the particles, the distance between their center of mass and the third particle, the angle between these two directions and three remaining angles defining the orientation of the total system. The latter three are rotational degrees of freedom and they define a plane containing the three α particles. The wavefunction of a 0^+ state is independent of these rotational coordinates. It depends upon the first three variables, which define a triangle with α particles in the corners. To visualize the shape of the state we sample a sequence of these triangles from the density distribution. That is in this sequence the number of triangles of a certain shape is proportional to the absolute square of the wavefunction of the set of coordinates corresponding to this triangle.

We then calculate the positions of the alpha particles for each set of coordinates in the sequence and mark them as points on a plot. The distribution of these points reflects the spatial structure of the corresponding state. The frame in which the positions of alpha particles are plotted is chosen in the following way: i) the center of mass of the system is positioned in the center of the plot; ii) the system is oriented so that two of the three particles are in the lower halfplane and the last particle is in the upper halfplane; iii) one of the two principal axes of inertia is aligned vertically. Note that the condition (ii) introduces certain up-down asymmetry. For simplicity the origin of the system of coordinates on

the plot is put at the lower left corner.

The result is shown in fig. 2 for the ground state, which clearly resembles an equal side triangle – a consequence of the fact that the ground state contains predominantly the lowest and simplest angular eigenfunction. The corresponding contour plot for the excited state is shown in fig. 3. Unlike the ground state the excited state has larger contributions from the higher angular eigenfunctions. The structure is therefore a complicated interplay between different configurations with the tendency to add up to a somewhat elongated triangle.

In addition we calculate the maximum probability configuration. The latter for the ground state is close to an equal side triangle with the length of the sides equal to 2.98 fm. For the excited state it is a somewhat elongated triangle with the length of the sides equal to 3.9, 4.2, 6.1 fm.

Conclusion. We have formulated an approach to deal with the three-body Coulomb problem in the continuum. The approach is then applied to three interacting α -particles which gives a description of the lowest two 0^+ levels in ^{12}C . The second of these states is in the 3α -particle continuum held together by the Coulomb barrier. We construct adiabatic hyperradial potentials and estimate the width of the excited state by solving the system of hyperradial equations for the complex energy. The width, estimated for the first time consistently within the three-body model, is found to be 20 eV which is in good agreement with the experimental value proving the validity of the formulated approach. The model includes a genuine three-body force, which imitates off-shell effects or residual three-body interactions. Furthermore, the model constitutes an improvement over previous three-body calculations when we compare with measured values of the root mean square radius and the monopole transition matrix element. The spatial structure of the ground state is confirmed to be predominantly an equal side triangle while the excited state has a much broader probability distribution with a tendency to look like a flat triangle.

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Figure Captions

Figure 1 The effective potentials $W_n = ((\lambda_n + 15/4)/\rho^2 - Q_{nn})\hbar^2/(2m)$ for the three lowest adiabatic channels as functions of hyperradius. The dashed line represents the position of the 0_2^+ resonance.

Figure 2 Contour density plot of the ground state described in detail in the text. The unit on the axes is fm.

Figure 3 The same as in fig.2 for the excited state.

Table 1

Parameters and properties of the 0^+ states. The results of this work are given in the first row. The results from the calculations in ref. [11] and ref. [12] are given in the next two rows and the measured values are shown in the last row. We show the parameters (strength S_3 and range b_3) of the three-body interactions, which lead to the energies $E(0_i^+)$ of the two 0^+ states measured relative to the threshold of three free α -particles. Finally we show the root mean square radius R_{rms} of the ground state, the monopole matrix element M and the width Γ of the excited state.

	S_3 , MeV	b_3 , fm	$E(0_{gs}^+)$, MeV	R_{rms} , fm	$E(0_2^+)$, MeV	$\Gamma(0_2^+)$, eV	M , fm ²
this work	-96.8	3.9	-6.81	2.36	0.38	20	6.54
[11]	-	-	-6.60	2.63	-0.04	-	8.18
[12]	-	-	-14	2.68	-3	-	9.35
exp.	-	-	-7.25	2.47	0.38	8.3 ± 1.0	5.7

Figure 1





